We claim

5 1. A.3-heterocyclyl-substituted benzoyl derivative of the formula I

15

where the variables have the following meanings:

25 R3 is hydrogen, halogen or $C_1 \cdot C_6 \cdot alkyl$;

 R^4 , R^5 are hydrogen, halogen, cyano, nitro, C1-C4-alkyl, C_1-C_4 -alkoxy- C_1-C_4 -alkyl, di(C_1-C_4 -alkoxy)- C_1-C_4 alkyl, di $(C_1-C_4-alkyl)$ -amino- $C_1-C_4-alkyl$, 30 $[2,2-di(C_1-C_4-alkyl)-1-hydrazino]-C_1-C_4-alkyl,$ $C_1 - C_6 - alkyliminooxy - C_1 - C_4 - alkyl, C_1 - C_4 - alkoxycarbonyl C_1 - C_4 - alkyl$, $C_1 - C_4 - alkyl$ thio $- C_1 - C_4 - alkyl$, C₁-C₄-haloalkyl, C₁-C₄-cyanoalkyl, C₃-C₈-cycloalkyl, C_1-C_4 -alkoxy, C_1-C_4 -alkoxy- C_2-C_4 -alkoxy, 35 C₁-C₄-haloalkoxy, hydroxyl, C₁-C₄-alkylcarbonyloxy, C₁-C₄-alkylthio, C₁-C₄-haloalkylthio, di(C₁-C₄-alkyl)amino, COR⁶, phenyl or benzyl, it being possible for the two last-mentioned substituents to be fully or partially halogenated 40 and/or to have attached to them one to three of the following groups: nitro, cyano, C₁-C₄-alkyl, C₁-C₄-haloalkyl,

 C_1-C_4 -alkoxy or C_1-C_4 -haloalkoxy;

			104
	5	R ⁴ and R ⁵	together form a $C_2 \cdot C_6$ -alkanediyl chain which can be mono- to tetrasubstituted by $C_1 \cdot C_4$ -alkyl and/or which can be interrupted by oxygen or by a nitrogen which is unsubstituted or substituted by $C_1 \cdot C_4$ -alkyl;
		or	
	10	R ⁴ and R ⁵	together with the corresponding carbon form a carbonyl or thiocarbonyl group;
	15	R ⁶	is hydrogen, C_1 - C_4 -alkyl, C_1 - C_4 -haloalkyl, C_1 - C_4 -alkoxy, C_1 - C_4 -alkoxy- C_2 - C_4 -alkoxy, C_1 - C_4 -haloalkoxy, C_3 - C_6 -alkenyloxy, C_3 - C_6 -alkynyloxy or NR^7R^8 ;
		R ⁷	is hydrogen or C ₁ -C ₄ -alkyl;
	20	R ⁸	is C ₁ -C ₄ -alkyl;
		Х	is O, S, NR ⁹ , CO or CR ¹⁰ R ¹¹ ;
i i	25	Y	is O, S, NR ¹² , CO or CR ¹³ R ¹⁴ ;
		R ⁹ , R ¹²	are hydrogen or C ₁ -C ₄ -alkyl;
	30	R ¹⁰ , R ¹¹ ,	R^{13} , R^{14} are hydrogen, C_1 - C_4 -alkyl, C_1 - C_4 -haloalkyl, C_1 - C_4 -alkoxycarbonyl, C_1 - C_4 -haloalkoxycarbonyl or $CONR^7R^8$;
		or	
	35	R ⁴ and R ⁹	or R^4 and R^{10} or R^5 and R^{12} or R^5 and R^{13} together form a C_2 - C_6 -alkanediyl chain which can be monot tetrasubstituted by C_1 - C_4 -alkyl and/or interrupted by oxygen or by a nitrogen which is unsubstituted
	40	•	or substituted by C ₁ -C ₄ -alkyl;
		R ¹⁵	is a pyrazole of the formula II which is linked in the 4-position

ΙI

where

10

5

 R^{16} is $C_1 \cdot C_6 \cdot alkyl;$

Z

R17

is H or SO_2R^{17} ;

15

20

is C₁-C₄-alkyl, C₁-C₄-haloalkyl, phenyl or phenyl which is partially or fully halogenated and/or has attached to it one to three of the following groups: nitro, cyano, C₁-C₄-alkyl, C₁-C₄-haloalkyl, C₁-C₄-alkoxy or C₁-C₄-haloalkoxy;

is hydrogen or C₁-C₆-alkyl;

25

where X and Y are not simultaneously sulfur;

with the exception of

 $\begin{tabular}{ll} 4- & [2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonyl-benzoyl]-1-ethyl-5-hydroxy-1H-pyrazole, \end{tabular}$

- 4-[2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonyl-benzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole,
 4-[2-chloro-3-(5-cyano-4,5-dihydroisoxazol-3-yl)-4-methyl-sulfonylbenzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole,
 4-[2-chloro-3-(4,5-dihydrothiazol-2-yl)-4-methylsulfonyl-
- benzoy1]-1,3-dimethyl-5-hydroxy-1H-pyrazole and
 4-[2-chloro-3-(thiazoline-4,5-dion-2-yl)-4-methylsulfonylbenzoy1]-1,3-dimethyl-5-hydroxy-1H-pyrazole;

or an agriculturally useful salt thereof.

- 2. A 3-heterocyclyl-substituted benzoyl derivative of the formula I where the variables have the following meanings:

```
\mathbb{R}^3
                           is hydrogen, halogen or C1-C6-alkyl;
        5
                R4, R5
                           are hydrogen, halogen, cyano, nitro, C1-C4-alkyl,
                           C_1 - C_4 - alkoxy - C_1 - C_4 - alkyl, di(C_1 - C_4 - alkoxy) - C_1 - C_4 - alkoxy
                           alkyl, di(C_1-C_4-alkyl)-amino-C_1-C_4-alkyl,
                           [2,2-di(C_1-C_4-alkyl)-l-hydrazino]-C_1-C_4-alkyl,
       10
                           C<sub>1</sub>-C<sub>6</sub>-alkyliminooxy-C<sub>1</sub>-C<sub>4</sub>-alkyl, C<sub>1</sub>-C<sub>4</sub>-alkoxycarbonyl-
                           C_1-C_4-alkyl, C_1-C_4-alkylthio-C_1-C_4-alkyl,
                           C1-C4-haloalkyl, C1-C4-cyanoalkyl, C3-C8-cycloalkyl,
                           C_1 \cdot C_4 \cdot alkoxy, C_1 \cdot C_4 \cdot alkoxy \cdot C_2 \cdot C_4 \cdot alkoxy,
                           C1-C4-haloalkoxy, C1-C4-alkylthio,
       15
                           C1-C4-haloalkylthio, di (C1-C4-alkyl) amino, COR6,
                           phenyl or benzyl, it being possible for the two
                           last-mentioned substituents to be fully or partially
                           halogenated and/or to have attached to them one to
                           three of the following groups:
       20
                           nitro, cyano, C1-C4-alkyl, C1-C4-haloalkyl,
                           C1-C4-alkoxy or C1-C4-haloalkoxy;
or
       25
                R4 and R5 together form a C2-C6-alkanediyl chain which can be
                              mono- to tetrasubstituted by C1-C4-alkyl and/or
                              which can be interrupted by oxygen or by a
                              nitrogen which is unsubstituted or substituted by
       30
                              C_1 \cdot C_4 \cdot alkyl;
                or
                              together with the corresponding carbon form a
       35
                              carbonyl or thiocarbonyl group;
                R6
                              is C_1 - C_4 - alkyl, C_1 - C_4 - haloalkyl, C_1 - C_4 - alkoxy,
                              C_1 - C_4 - alkoxy - C_2 - C_4 - alkoxy, C_1 - C_4 - haloalkoxy,
                              C<sub>3</sub>-C<sub>6</sub>-alkenyloxy, C<sub>3</sub>-C<sub>6</sub>-alkynyloxy or NR<sup>7</sup>R<sup>8</sup>;
       40
                \mathbb{R}^7
                              is hydrogen or C1-C4-alkyl;
                R8
                              is C<sub>1</sub>-C<sub>4</sub>-alkyl;
       45
```

3-Heterocyclyl-substituted benzoyl derivatives

_ Abstract

Benzovl derivatives of the formula I

where the variables have the following meanings:

20 R¹, R² are hydrogen, nitro, halogen, cyano, alkyl, haloalkyl, alkoxy, haloalkoxy, alkylthio, haloalkylthio, alkylsulfinyl, haloalkylsulfinyl, alkylsulfonyl or C₁-C₆-haloalkylsulfonyl;

25 R^3 is hydrogen, halogen or alkyl;

R4, R5 are hydrogen, halogen, cyano, nitro, alkyl, alkoxy, alkylthio, dialkylamino, phenyl or carbonyl, it being possible for the 6 last-mentioned radicals to be substituted;

X is O, S, NR^9 , CO or $CR^{10}R^{11}$;

Y is O, S, NR^{12} , CO or $CR^{13}R^{14}$;

is pyrazole which is unsubstituted or substituted, linked in the 4-position and has attached to it in the 5-position a hydroxyl or sulfonyloxy radical;

and the agriculturally useful salts thereof; processes and intermediates for the preparation of the 3-heterocyclyl-substituted benzoyl derivatives; compositions comprising them; and the use of these derivatives or compositions comprising them for controlling undesirable plants.

where X and Y are not simultaneously oxygen or sulfur;

with the exception of

- 4-[2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl]-1-ethyl-5-hydroxy-1H-pyrazole,
 - 4-[2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonyl-benzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole,
 - 4-[2-chloro-3-(5-cyano-4,5-dihydroisoxazol-3-yl)-4-methyl-sulfonylbenzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole,
- 4-[2-chloro-3-(4,5-dihydrothiazol-2-yl)-4-methylsulfonyl-benzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole and
 4-[2-chloro-3-(thiazoline-4,5-dion-2-yl)-4-methylsulfonyl-benzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole;
- or an agriculturally useful salt thereof.
 - A 3-heterocyclyl-substituted benzoyl derivative of the formula I as claimed in claim 1 or 2, where R³ is hydrogen.

20

4. A 3-heterocyclyl-substituted benzoyl derivative of the formula I as claimed in any of claims 1 to 3, where

25

- $\begin{array}{lll} R^1,R^2 & \text{are nitro, halogen, cyano, } C_1\text{-}C_6\text{-}alkyl, \\ & C_1\text{-}C_6\text{-}haloalkyl, } C_1\text{-}C_6\text{-}alkoxy, } C_1\text{-}C_6\text{-}haloalkyl, \\ & C_1\text{-}C_6\text{-}alkylthio, } C_1\text{-}C_6\text{-}haloalkylthio, \\ & C_1\text{-}C_6\text{-}alkylsulfinyl, } C_1\text{-}C_6\text{-}haloalkylsulfinyl, \\ & C_1\text{-}C_6\text{-}alkylsulfonyl or } C_1\text{-}C_6\text{-}haloalkylsulfonyl. \\ \end{array}$
- 5. A 3-heterocyclyl-substituted benzoyl derivative of the formula I as claimed in any of claims 1 to 4, where Z is ${\rm SO}_2R^{17}$.
- 35 6. A 3-heterocyclyl-substituted benzoyl derivative of the formula I as claimed in any of claims 1 to 4, where Z is hydrogen.
- A 3-heterocyclyl-substituted benzoyl derivative of the formula I as claimed in any of claims 1 to 4 or 6, where X is oxygen and Y is CR¹³R¹⁴.
 - 8. A 3-heterocyclyl-substituted benzoyl derivative of the formula I as claimed in any of claims 1 to 4 or 6 or 7, where

	- 4	1 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
	R ⁴	is halogen, nitro, C ₁ -C ₄ -alkyl,
		$C_1 - C_4 - alkoxy - C_1 - C_4 - alkyl$,
		$C_1-C_4-alkoxycarbonyl-C_1-C_4-alkyl$,
		$C_1-C_4-alkylthio-C_1-C_4-alkyl, C_1-C_4-haloalkyl,$
5		C_1 - C_4 -cyanoalkyl, C_3 - C_8 -cycloalkyl, C_1 - C_4 -alkoxy,
		C_1-C_4 -alkoxy- C_2-C_4 -alkoxy, C_1-C_4 -haloalkoxy,
		C_1 - C_4 -alkylthio, C_1 - C_4 -haloalkylthio,
		di(C ₁ -C ₄ -alkyl)amino, COR ⁶ , phenyl or benzyl, it
		being possible for the two last-mentioned
10		substituents to be partially or fully halogenated
		and/or to have attached to them one to three of
		the following groups:
		nitro, cyano, C ₁ -C ₄ -alkyl, C ₁ -C ₄ -haloalkyl,
		C ₁ -C ₄ -alkoxy or C ₁ -C ₄ -haloalkoxy;
15		
	-5	de budanaman on C. C. oller).
	R ⁵	is hydrogen or C ₁ -C ₄ -alkyl;
	or	
20		
20	\mathbb{R}^4 and \mathbb{R}^5	together form a C2-C6-alkanediyl chain which can be
		mono- to tetrasubstituted by C ₁ -C ₄ -alkyl and/or
		which can be interrupted by oxygen or by a
		nitrogen which is unsubstituted or substituted by
		C ₁ -C ₄ -alkyl;
25		01 04 42.4727
	or	
• •	R^5 and R^{13}	together form a C_2 - C_6 -alkanediyl chain which can be
30		mono- to tetrasubstituted by C_1 - C_4 -alkyl and/or
		which can be interrupted by oxygen or by a
		nitrogen which is unsubstituted or substituted by
		C ₁ -C ₄ -alkyl.
35 9	. A 3-hetero	ocyclyl-substituted benzoyl derivative of the
-		as claimed in any of claims 1 to 4 or 6 to 8, where
	-4	de o o allud o o haleslind
	R ⁴	is C ₁ -C ₄ -alkyl, C ₁ -C ₄ -haloalkyl,
40		C ₁ -C ₄ -alkoxycarbonyl or CONR ⁷ R ⁸ ;
	R ⁵	is hydrogen or C ₁ -C ₄ -alkyl;
	or	
45		
		. •

R4 and R5 together form a C₂-C₆-alkanediyl chain which can be mono- to tetrasubstituted by C₁-C₄-alkyl and/or which can be interrupted by oxygen or by a nitrogen which is unsubstituted or substituted by C₁-C₄-alkyl;

or

5

R5 and R13 together form a $C_2 \cdot C_6$ -alkanediyl chain which can be mono- to tetrasubstituted by $C_1 \cdot C_4$ -alkyl and/or which can be interrupted by oxygen or by a nitrogen which is unsubstituted or substituted by $C_1 \cdot C_4$ -alkyl.

- 20 11. A 3-heterocyclyl-substituted benzoyl derivative of the formula I as claimed in any of claims 1 to 4 or 6 or 7 or 10, where R¹⁸ is hydrogen.
- 12.4-[2-Chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonyl-benzoyl]-1-methyl-5-hydroxy-1H-pyrazole.
 - 13. An agriculturally useful salt of 4-[2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl]-1-methyl-5-hydroxy-1H-pyrazole.

30

- 14. A 3-heterocyclyl-substituted benzoyl derivative of the formula I as claimed in any of claims 1 to 4 or 6, where
- 35 X is S, NR^9 , CO or $CR^{10}R^{11}$;

or

Y is O, S, NR^{12} or CO.

40

15. A 3-heterocyclyl-substituted benzoyl derivative of the formula I as claimed in any of claims 1 to 4 or 6 or 14, where \mathbb{R}^{18} is hydrogen.

16. A 3-heterocyclyl-substituted benzoyl derivative of the formula I as claimed in any of claims 1 to 4 or 6 or 14, where

```
5
       R4
                    is halogen, cyano, nitro, C1-C4-alkyl,
                    C_1 - C_4 - alkoxy - C_1 - C_4 - alkyl,
                    C_1 - C_4 - alkoxycarbonyl - C_1 - C_4 - alkyl,
                    C_1-C_4-alkylthio-C_1-C_4-alkyl, C_1-C_4-haloalkyl,
                    C1-C4-cyanoalkyl, C3-C8-cycloalkyl, C1-C4-alkoxy,
10
                    C_1-C_4-alkoxy-C_2-C_4-alkoxy, C_1-C_4-haloalkoxy,
                    C1-C4-alkylthio, C1-C4-haloalkylthio,
                    di(C1-C4-alkyl)amino, COR6, phenyl or benzyl, it
                    being possible for the two last-mentioned
                    substituents to be partially or fully halogenated
15
                    and/or to have attached to them one to three of
                    the following groups:
                    nitro, cyano, C1-C4-alkyl, C1-C4-haloalkyl,
                    C1-C4-alkoxy or C1-C4-haloalkoxy;
```

20 R⁵ is hydrogen or C_1-C_4 -alkyl;

or

25 R^4 and R^5 together form a $C_2 \cdot C_6 \cdot$ alkanediyl chain which can be mono- to tetrasubstituted by $C_1 \cdot C_4 \cdot$ alkyl and/or which can be interrupted by oxygen or by a nitrogen which is unsubstituted or substituted by $C_1 \cdot C_4 \cdot$ alkyl;

30

45

or

R4 and R9 or R4 and R10 or R5 and R12 or R5 and R13 together form a C_2 - C_6 -alkanediyl chain which can be mono- to tetrasubstituted by C_1 - C_4 -alkyl and/or which can be interrupted by oxygen or by a nitrogen which is unsubstituted or substituted by C_1 - C_4 -alkyl;

40 R^{18} is C_1-C_6 -alkyl.

17. A process for the preparation of 3-heterocyclyl-substituted benzoyl derivatives of the formula I as claimed in claim 1, which comprises acylating the pyrazole of the formula II where Z = H, where the variables R¹⁶ and R¹⁸ have the meanings given under claim 1,

10

15

20

25

30

i M

$$R^{18}$$
 $N \sim N$
 OH
 R^{16}

II (where $Z = H$)

with an activated carboxylic acid III α or with a carboxylic acid III β ,

where the variables R^1 to R^5 , X and Y have the meanings given under claim 1 and L^1 is a nucleophilically displaceable leaving group, subjecting the acylation product to a rearrangement reaction in the presence or absence of a catalyst to give the compounds I (where Z = H) and, if desired, to prepare 3-heterocyclyl-substituted benzoyl derivatives of the formula I where Z = SO_2R^{17} , reacting the product with a compound of the formula V,

$$L^2$$
 SO₂R¹⁷ V

where \mathbb{R}^{17} has the meaning given under claim 1 and \mathbb{L}^2 is a nucleophilically displaceable leaving group.

18. A 3-heterocyclyl-substituted benzoic acid derivative of the formula III,

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15

vl)benzoate.

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where R¹⁹ is hydroxyl or a radical which can be removed by hydrolysis and variables R¹ to R⁵, X and Y have the meanings given under the claims 1 to 16, with the exception of methyl 2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonyl-benzoate, methyl 2-chloro-3-(4,5-dihydrooxazol-2-yl)-4-methylsulfonylbenzoate and methyl 2,4-dichloro-3-(5-methylcarbonyloxy-4,5-dihydroisoxazol-3-

19. A 3-heterocyclyl-substituted benzoic acid derivative of the formula III as claimed in claim 18 where the variables R^1 to R^5 , X and Y have the meanings given under claims 2 to 16.

25 20. A 3-heterocyclyl-substituted benzoic acid derivative of the formula III as claimed in either of claims 18 or 19, where

 R^{19} is halogen, hydroxyl or C_1 - C_6 -alkoxy.

30 21. A composition comprising a herbicidally active amount of at least one 3-heterocyclyl-substituted benzoyl derivative of the formula I or of an agriculturally useful salt of I as claimed in any of claims 1 to 16, and auxiliaries conventionally used for the formulation of crop protection products.

22. A process for the preparation of a composition as claimed in claim 21, which comprises mixing a herbicidally active amount of at least one 3-heterocyclyl-substituted benzoyl derivative of the formula I or of an agriculturally useful salt of I as claimed in any of claims 1 to 16 and auxiliaries conventionally used for the formulation of crop protection products.

23. A method of controlling undesirable vegetation, which comprises allowing a herbicidally active amount of at least one 3-heterocyclyl-substituted benzoyl derivative of the

formula I or of an agriculturally useful salt of I as claimed in any of claims 1 to 16 to act on plants, their environment and/or on seeds.

5 24. The use of a 3-heterocyclyl-substituted benzoyl derivative of the formula I or an agriculturally useful salt thereof as claimed in any of claims 1 to 16 as herbicide.